

Supplementary data

Table S1 MP2/6-311+G(2df) Optimised coordinates of complexes **1** and **2**.

1	x	y	z	2	x	y	z
C	-2.05614	0.65696	0.614402	C	0	1.391657	-0.90505
H	-2.61699	1.464442	1.071285	H	0	2.475559	-0.90536
C	-0.62412	-1.42427	-0.55999	C	0	-1.39166	-0.90505
H	-0.05539	-2.227	-1.01474	H	0	-2.47556	-0.90536
C	-1.34119	-0.53556	-1.35711	C	1.20609	-0.69583	-0.90936
H	-1.34188	-0.65463	-2.43457	H	2.144458	-1.23821	-0.91286
C	-0.63187	-1.27824	0.825639	C	-1.20609	-0.69583	-0.90936
H	-0.07766	-1.97549	1.443618	H	-2.14446	-1.23821	-0.91286
C	-2.05693	0.505254	-0.77044	C	1.20609	0.695826	-0.90936
H	-2.61668	1.196005	-1.39067	H	2.144458	1.238207	-0.91286
C	-1.34776	-0.23864	1.413237	C	-1.20609	0.695826	-0.90936
H	-1.35783	-0.12818	2.491665	H	-2.14446	1.238207	-0.91286
C	0.950641	2.031309	0.06186	C	0	0.66569	2.3848
C	1.559787	0.986114	-0.50912	C	0	-0.66569	2.3848
H	0.956816	2.149484	1.138717	H	-0.92262	1.229282	2.382416
H	0.439607	2.785677	-0.51927	H	0.922622	1.229282	2.382416
H	1.574763	0.831541	-1.58113	H	0.922622	-1.22928	2.382416
C	2.245318	-0.00508	0.323495	H	-0.92262	-1.22928	2.382416
O	2.839313	-0.97732	-0.10864				
H	2.194332	0.189613	1.412282				